1 of 1

Technical Progress Report
For Second Year Efforts Related To
Project Entitled:
HYDRODYNAMIC CONTROLS ON PARTICLE TRANSPORT THROUGH
HETEROGENEOUS POROUS MEDIA

PI: DR. STEPHEN E. SILLIMAN

CO-PI: DR. MARIJAN BABIC

BOTH AT:

DEPT. OF CIVIL ENGINEERING AND GEOLOGICAL SCIENCES
UNIVERSITY OF NOTRE DAME
NOTRE DAME, INDIANA 46556

Date of Submission: September 28, 1993

MASTER

ABSTRACT

The University of Notre Dame is investigating the hydrodynamic controls on particle transport through heterogeneous porous media. A number of research initiatives have been pursued, including: (i) experiments on two-dimensional, saturated media, (ii) experiments on three-dimensional, saturated media, (iii) development of an apparatus for experiments in converging or diverging flow fields, (iv) use of a UV curing resin for "freezing" flow, (v) Hele-Shaw experiments on complex geometries, (vi) solution to the Navier-Stokes equation (verified through the Healy-Shaw efforts), (vii) utilization of random field generators for simulating structure in sediments, (viii) experiments in unsaturated media, and (ix) the use of MODFLOW to analyze flow in experiments. Results to date include: (i) large latex spheres (>7 microns) are preferentially held within the medium as compared to smaller latex spheres (<7 microns) and are concentrated near changes in pore size, (ii) the degree to which latex spheres remain within the medium does not appear to be altered through lowering the ionic strength of the pore fluid, (iii) the number spheres remaining in the medium is a function of the hydraulic heterogeneity, (iv) the number of spheres remaining within the medium decreases when the carrying fluid is the UV curing resin (200 cP) as compared to when the carrying fluid is salt water, (v) the UV curing resin represents a significant new tool for capturing transport behavior in both saturated and unsaturated systems, (vi) qualitative comparison of the Hele-Shaw and numerical efforts indicate general agreement, and (vii) permeability and dispersivity studies are providing interesting relationships for the simulated media. Extensions will include particle transport experiments in 3-D and converging / diverging flow fields, addition of particles to the Hele-Shaw models, numerical simulation of particle transport through simulated media, and extension of the study of unsaturated flow. In addition, some redirection of research will occur to respond to collaborations with the Heterogeneity Subprogram, new projects in the SSP, and investigators working with microbial transport.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

RECEIVED
OCT 13 1993
CSTI

RESEARCH PURPOSE

Sophisticated models of the movement of particles, particularly bacteria and viruses, through porous media have been developed, but have met with limited success when compared to field observations (e.g. Harvey et al., 1989, 1993). Mills et al. (1990) argue that the poor predictive capabilities of the models are due in part to the fact that most of the sophisticated models are tied to an assumptions of homogeneity within the flow field. This argument is supported by the recent field efforts of Harvey et al. (1993).

In previous work, Silliman (1990) has investigated the structure of random percolation fields and has suggested application of percolation theory to heterogeneous porous media. One conclusion from this study as applied to particle transport is that as the distribution of pore throat sizes takes on variation in the third dimension, the probability of finding a continuous flow path with large throat size increases. One interpretation of this work, within the current context, leads to an argument that a saturated medium will become more open to transport of particles as the medium takes on three dimensional structure.

The central hypothesis of the current project is therefore be stated:

Particles which are suspended within the pore fluids of media demonstrating three-dimensional heterogeneities will be transported at higher average velocities and with less trapping than particles which are suspended in the pore fluids of media demonstrating one- or two-dimensional heterogeneities. This dependence on dimension is a function of the dimensional character of the heterogeneity, the length scales of the heterogeneity, the size of the particles, the hydrodynamics of the flow field, the degree of saturation of the medium, and the medium/particle interaction.

LITERATURE REVIEW

The movement of particles within porous media is of importance in many scientific and engineering applications including control of disease, contamination of groundwater, bioremediation of groundwater, reduction of primary permeability via clay mobility, and secondary recovery of oil or minerals derived from solution mining (McCarthy and Degueudre, 1993; Mills et al., 1991; McCarthy and Zachara, 1989). Particles which may be of interest in these applications include clays, silicates, iron or aluminum oxides, bacteria, viruses, humic matter from the unsaturated zone, calcite and iron sulfates, and artificially introduced particles.

Among the controls on the movement of a particle are the density, motility, size and surface chemistry of the particle. Also important are the flow rate through the medium and the chemistry/ viscosity of the transport fluid. The transport of the particles can be reduced and/or eliminated through several mechanisms including filtration, physicochemical attraction to the stationary phase of the medium, flocculation, biological interaction and changes in water chemistry (Mills et al., 1991; McCarthy and Zachara, 1989; McDowell-Boyer et al., 1986). Recent work by Dr. Silliman (unpublished) and Wilson et al. (1993) also indicate that interfaces in unsaturated systems may also play key roles in reducing the advective motion of particles.

Both experimental and theoretical studies have indicated the importance of heterogeneity on particle transport. Mills et al. (1990) demonstrated the influence of media heterogeneity in an experimental medium consisting of a low permeability matrix containing a discrete, high-permeability flow path. More recently, Harvey et al. (1993) have reported a series of experiments, both in columns and in the field, involving transport of a conservative tracer, inert microparticles, and bacteria. These authors concluded that the mechanisms influencing the transport of the particles in the field (adsorption) were different than those in the laboratory (physical straining), but also concluded that at the field and laboratory scale, physical heterogeneity was an important factor in the movement of the particles and bacteria.

As noted in the previous section, previous work by Silliman (1990) has demonstrated from a mathematical standpoint that the structure of random fields (in particular, percolation clusters) was dependent to a large degree on the dimension of the random field. Our interpretation of this theoretical work, in combination with the review of the experimental work on particle transport through porous media, leads to the conclusion that a saturated medium will become more open to transport of particles as the dimensionality of the medium increases.

RESEARCH OBJECTIVES

Based on the literature review presented, and our initial results, we suggest an extension of the work by Mills et al. (1990) through laboratory and theoretical experiments investigating the hydrodynamic mechanisms influencing particle transport through saturated and partially saturated porous media. In particular, we propose a series of intermediate-scale experiments in which the same porous materials are packed in two- and three-dimensional arrays of heterogeneity and a series of numerical efforts focused on scaling of microscale transport mechanisms.

Specific objectives of these efforts include:

(i) Determine the dependence of particle transport on medium heterogeneity. Specifically, how will the rate of travel of particles and percent of particles being trapped within the column depend on the size and dimension of heterogeneities,

- (ii) Utilizing direct observation and destructive sampling, identify the paths taken by different sized particles in the presence of heterogeneities,
- (iii) Develop a data base on the hydrodynamic behavior of the particles during transport,
- (iv) Investigate the dependence of transport on the length scale of the heterogeneity.
- (v) Investigate the dependence of transport characteristics on degree of saturation,
- (vi) Determine the macroscopic applicability of advection-dispersion models of particle transport through comparison of results for the chemical and particle tracers,
- (vii) Provide a foundation for improvement of the mathematical description of particle transport through comparison of results for the particle tracers with ongoing numerical efforts, and
- (viii) Further develop an innovative methodology for destructive sampling of laboratory cores which allows detailed examination of the location of particles during transport.

RESEARCH APPROACH

Construction of Flow Cells for 2-D and 3-D Experiments

The laboratory design used in this work involves the use of a series of flow cells designed to allow injection to the experimental medium at a constant rate and maintenance of a constant hydraulic head at the outflow from the medium. Recirculation loops are maintained at the inflow and outflow reservoirs to allow mixing within both reservoirs. Finally, sampling ports are provided at the inflow and outflow ends of the flow cell.

Shown in Figure 1, the general schematic of the flow cell is based on a confined system. Details on the construction of these flow cells may be found in a white paper to be distributed within the Subsurface Science Program (Silliman, 1993, in revision). The use of plexiglass has provided optimal opportunity for visual inspection of the flow within the experimental medium and was critical in our initial efforts to minimize short-circuit flow along the walls of the tank. The absolute dimensions of flow cells already constructed vary from a minimum of approximately 36 cm x 18 cm x 5 cm to a current maximum of approximately 61 cm x 30 cm x 20 cm. It is anticipated that a larger flow cell will be constructed during the coming year (with emphasis on enlargement of the third dimension relative to the length of the cell). It was decided to utilize a confined system to minimize contamination and facilitate comparison with flow cells utilized at SERF (the research facility at Pacific Northwest Laboratories).

Flow along the top and bottom surface of the flow cell has been minimized through use of a plastic lattice consisting of open squares approximately one centimeter on a side with a depth of approximately one centimeter. This lattice has effectively eliminated edge flow along the most sensitive surfaces.

This flow cell design has been utilized in a series of experiments on two-dimensional media (as discussed later in this packet) and is currently being utilized to complete the first of the three-dimensional experiments. To date, these cells have served us very well by providing controllable experiments, maximizing visual inspection, and minimizing cost. Cost of these cells, excluding laboratory labor time, ranges from approximately \$300 to approximately \$800 depending on size of the flow cell.

Running Experiments in 2- and 3-Dimensional Media: Tracers and Carrying Fluids

To date, all experiments in the two-dimensional flow fields have utilized both latex

particles and colored water as tracers. The colored water has provided rapid visual inspection of the movement of the tracer front within the medium, a rapid visual check for density effects, a means of determining whether a particular medium was properly packed to avoid edge effects, and a general idea of arrival times and dispersion. The latex particles (no carboxylate groups added but fluorescence used in all experiments to date) have ranged in size from approximately 2 microns to approximately 80 microns. This size range of the latex spheres was chosen for a number of reasons including:

- (i) the large size reduces the influence of surface interactions and adsorption, thus selecting hydrodynamic stresses and gravity as the primary forces influencing particle motion,
- (ii) larger particles are less influenced by weak forces such as diffusion, and
- (iii) these large spheres were chosen for ease of detection (extension to smaller particles should be possible through interaction with other research groups).

Two fluids have been utilized as the carrying fluid for the experiments. The first, water, is modified with sodium chloride to match the density of the particles. The second fluid utilized is a resin which cures under exposure to UV light. Discussed in the section on scientific accomplishments, the goal of the use of this resin is to allow local "freezing" of pore fluids to allow direct inspection of particle transport at particular locations and times. This resin also has a significantly higher viscosity than water, allowing direct analysis of the research questions related to the influence of hydrodynamic forces on particle transport.

Results from each experiment are collected in two fashions. First, outflow samples are collected at regular time intervals. These samples are characterized based on total particle counts and size distribution. Second, after the system has been flushed sufficiently that no additional particles are observed in the outflow, the flow field is stopped and the experimental medium is sampled to determine particle concentration trapped within the medium. For the experiments using water, this sampling is performed by opening the flow cell and collecting samples of the medium manually. For experiments involving the resin, selected locations within the medium are first frozen through exposure to UV light. The flow cell is then opened, the cured pieces of the medium are removed for analysis and selected locations in uncured portions of the medium are manually sampled.

As the experiments progress into three-dimensional media, chemical tracers will be used to help define the details of the hydrodynamic dispersion. This becomes necessary as direct observation of dye tracers is not possible. It is also anticipated that selected 2-dimensional experiments will be duplicated with chemical tracers both to establish reproducibility and to provide quantified data sets on hydrodynamic dispersion.

Figure 1: Simple Schematic of Flow Cell Design for Saturated Systems

Results from each experiment are collected in two fashions. First, outflow samples are collected at regular time intervals. These samples are characterized based on total particle counts and size distribution. Second, after the system has been flushed sufficiently that no additional particles are observed in the outflow, the flow field is stopped and the experimental medium is sampled to determine particle concentration trapped within the medium. For the experiments using water, this sampling is performed by opening the flow cell and collecting samples of the medium manually. For experiments involving the resin, selected locations within the medium are first frozen through exposure to UV light. The flow cell is then opened, the cured pieces of the

medium are removed for analysis and selected locations in uncured portions of the medium are manually sampled.

As the experiments progress into three-dimensional media, chemical tracers will be used to help define the details of the hydrodynamic dispersion. This becomes necessary as direct observation of dye tracers is not possible. It is also anticipated that selected 2-dimensional experiments will be duplicated with chemical tracers both to establish reproducibility and to provide quantified data sets on hydrodynamic dispersion.

Running Experiments in 2- and 3-Dimensional Media: Experimental Media

All experiments run to date and all experiments anticipated in the near future will be run utilizing technical quality glass beads and/or Ottawa sand as the medium. These media are consistent with our desire to isolate the hydrodynamic forces influencing particle transport as they allow use of a range of ionic strengths in the carrying fluid (and use of the resin) without concern of mobilizing clay or other colloids within the medium. Further, use of these relatively non-cohesive materials allows reproducible packing of relatively complex heterogeneities. Finally, these materials improve our visualization and the cure of the UV resin (the depth of cure is a direct function of the depth of penetration of the UV light).

Figure 2 shows three of the heterogeneous media created for experiments in this project. Packing of flow cells involves careful addition of thin layers of glass beads (or sand) to mimic the desired distribution of heterogeneities. In addition to creating lens and layers of differing materials, we have been experimenting with the creation of stringers (thin fingers of one material cutting through a second material) through the movement of steel plates during the packing process. We have not yet perfected a technique to create distributions of hydraulic properties which change in a gradual rather than an abrupt manner.

A second major challenge to be addressed in our continuing efforts is the choice of what heterogeneities to consider. To date, we have based our conductivity distributions on structures of interest in terms of connectivity of conductivity zones. However, as the Subsurface Science Program becomes increasingly involved in field characterization, it is anticipated that our selection of heterogeneity structure will become more closely tied to field observation of structure and hypotheses generated in the field efforts.

Running Experiments in Converging / Diverging Flow Field

An innovative new flow cell design has been incorporated into this project. The purpose of this flow cell is to allow experiments to be run in which the average flow direction is either converging towards a well or diverging from a well. The essence of this design is the use of a 24" well screen as the outer screen on the flow cell and a 1" well screen as the inner screen. The experimental medium is placed between the screens. The two screens are bordered on the top and bottom by plexiglass plates such that there is a small reservoir on the interior of the 1" screen and a rather large reservoir around the exterior of the 24" screen. A general schematic of this design and further discussion of its attributes is given below in the section on scientific accomplishments.

Figure 2: Three Examples of Heterogeneities Utilized in Project.

Numerical Study of Particle Transport in Random Porous Media

Improved predictive ability at the macroscale and megascale may require an improved understanding of the interaction of forces at the microscopic scale. Towards this end, numerical modeling is being carried out on fluid flow, dispersion and particle transport through two dimensional representations of porous media structure. The goal of this effort is to further our understanding of the microscopic processes which influence macroscopic particle transport characteristics.

The numerical approach is carried out in three stages. The first stage utilizes numerical modelling to simulate fluid flow and streaklines through porous media generated using standard random field generators (turning bands, nearest neighbors and discrete analysis). The model, a Marker and Cell (MAC) finite difference approach, is based on the Navier-Stokes equation as applied to rectangular regions consisting of a mixture of open pores and solids. The medium is assumed to be periodic and the solution is completed over one unit cell. Among the products anticipated from this effort is a theoretical relationship between porosity and permeability for these simulated media.

The second stage of this effort involves analysis of the dispersive properties of the simulated media through homogenization theory. Typically, porous media are characterized by microstructure length scales which are much smaller than the macroscopic length scale of interest. Governing equations, written at the micro-length scale, have to be transformed before applying at the macroscale. In transformation from one scale to another, quantities at the microscale are averaged and used to describe phenomena at the macroscale. Through length scale transformation of the advection-diffusion equation a dispersion tensor can be obtained. The *homogenization method* is a way of averaging which exploits two geometrical properties. The first property is that porous media have two vastly different length scales (micro and macro) and the second one is a periodic microstructure. The media simulated in this study have both of these properties and are thus suitable for application of the homogenization theory. The homogenization theory is based on a double-scale asymptotic expansion, where the relevant scales are the micro-length scale l and the macro-length scale L . The length scale ratio $\epsilon = l/L$, is assumed to be a small parameter. After introducing the double-scale expansion in the governing microscopic equations and grouping equal powers of ϵ , a series of equations is obtained. The macroscopic equations can be obtained by taking the limit $\epsilon \rightarrow 0$. This process gives the passage from the microscopic description to macroscopic.

In our study, the homogenization method provides a simple means of calculating the dispersion tensor given the geometry of the unit periodic cell (the size of the simulated medium) and the velocity distribution within the pores. The solution obtained in this way can be compared to the direct solution of the advection-diffusion equation for the concentration at the microscale. The advantage of the homogenization approach is that the dispersion tensor can be obtained directly, rather than through fitting the average concentration profile to the corresponding analytical solution of the one-dimensional advection-dispersion equation.

The third stage involves utilizing Discrete Element Modelling (DEM) to follow particles through the simulated media. DEM allows estimation of trajectories of each of a large number of finite-mass particles moving through the simulated medium based on consideration of the various forces influencing each particle. These forces include body forces, hydrodynamic forces, and stochastic Brownian forces and their relative importance is a function of the particle Reynold's number and the particle Peclet number. These forces are numerically integrated to provide predicted paths, collisions with other particles and collisions with the medium. The goal of this

effort (as stated previously) is to provide a connection between the details of microscopic transport and the mathematical description of the macroscopic expression of that transport.

Hele-Shaw Cells for Calibration / Verification of Numerical Effort

Hele-Shaw type flow cells are being utilized to address the question of calibration and verification of the numerical effort in microscopic flows. Constructed as shown in Figure 3, these models provide a controlled environment from which to experimentally simulate flow through a complex pattern of open pores and solids. The design of these is quite simple with an upper plexiglass plate separated from a lower plexiglass plate by 1/8 inch thick plexiglass. The 1/8 inch plexiglass is cut to form both the outer boundaries of the flow field and a series of unconnected solid regions within the flow field.

Through use of a triple injection port, the flow through the cell can be controlled with respect to total flow and distribution of flow from the two outside injection ports. Through injection of dye at the center port, a cluster of flow lines can be traced through the cell. Use of plexiglass for the upper and lower plates combined with superposition of a grid under the flow cell allows accurate characterization of the traced flow lines through simple photography.

Provided with characterization of the experimental conditions (flow rate, temperature, flow lines selected, etc.), results in terms of pressure drop and flow line characteristics can be compared with results predicted by the numerical model.

Figure 3: Schematic of Hele-Shaw Model for Flow Through Complex Medium.

Experiments in Unsaturated Media

An initial design has been developed for running experiments in unsaturated media. This design allows addition of fluid to the upper surface of an unsaturated medium with collection from drains at the bottom of the medium. This apparatus provides the potential to run a series of experiments in which pulses of water are added to the surface, simulating infiltration events following precipitation.

The research will eventually incorporate an experimental design in which steady, unsaturated flow is maintained. The reasons for this extension are many and include:

- (i) Improved control of where the flow is moving,
- (ii) Improved reproducibility, and
- (iii) Better reliability in characterization of medium properties.

The current experiments are directed towards the hypothesis that zones with large pores (high conductivity in saturated conditions) will behave as conduits for transport at high infiltration rates, but will act as hindrances to transport at low infiltration rates. It is anticipated that this hypothesis will be addressed over the coming 4 months. Upon completion of this portion of the experiment, we anticipate extending this work to steady, unsaturated flow. These latter experiments will allow more detailed analysis of where the particles move in an unsaturated system, what the controlling factors are, and at what moisture contents different flow conduits become principal conduits of flow and/or transport.

Hydraulic characterization during the initial unsaturated experiments will be difficult. During the latter stage experiments, distribution of moisture content will be measured directly through destructive sampling and/or light penetration methods.

Monte Carlo Simulation:

Monte Carlo simulation allows analysis of flow and transport in a series of random conductivity fields which are related via their statistical description. Based on turning bands, discrete analysis, and nearest neighbors (random field generators), a number of studies of transport in heterogeneous media are being pursued. These include the study of the variability of the capture zone around a well, the study of the difference in behavior of flow in media characterized by continuously varying conductivities (e.g. turning bands and nearest neighbors) versus flow in media characterized by discretely varying conductivities (e.g. discrete analysis), and simulation of the flow fields used in our laboratory experiments.

The primary tool utilized is MODFLOW, a finite difference package produced by the U.S. Geological Survey. This model is used in conjunction with MODPATH, a conjugate gradient solution algorithm produced by the U.S.G. S., and random field generators programmed at Notre Dame.

PRINCIPAL TASKS

The principal tasks associated with this project and the degree of completion as of this review may be summarized:

(i) Testing of flow cell design for running experiments in two and three dimensions (95% complete),

(ii) Complete a series of particle and dye tracer studies in two dimensions providing a baseline study from which to extend to three dimensions and converging / diverging flow fields (85% complete),

(iii) Design experimental procedure for "freezing" pore fluid during an experiment (95% complete),

(iv) Complete a series of particle, chemical, and dye tracer experiments in three dimensions (10% complete),

(v) Design flow cell for converging / diverging flow experiments (70% complete),

(vi) Complete a series of particle, chemical and dye tracer experiments in the converging / diverging flow fields (5% complete),

(vii) Complete a series of particle, chemical and dye tracer experiments in unsaturated media (10% complete),

(viii) Characterize the hydraulic properties of the unsaturated media (10% complete),

(ix) Complete Monte Carlo study of transport through heterogeneous random fields (60% complete),

(x) Complete Marker and Cell model for flow through simulated porous media (90% complete),

(xi) Develop numerical relationship between porosity and permeability for simulated media (70% complete),

(xii) Calibrate / verify numerical solution utilizing Hele-Shaw Cell (60% complete),

(xiii) Develop homogenization technique for determination of dispersion tensor in simulated media (70% complete),

(xiv) Add particle transport to numerical model allowing modelling of a large number of particles through simulated media (50% complete),

(xv) Develop research interactions with other investigators within the SSP to ensure adequate hypotheses, experimental design, choice of media, and plans for future efforts (ongoing), and

(xvi) Contribute to new Heterogeneity Subprogram and modify experimental designs to address primary hypotheses within this new subprogram (ongoing).

SCIENTIFIC PROGRESS TO DATE

Significant progress has been achieved in a number of the task areas. On the following pages, the primary accomplishments in the areas of the equipment development (including the resin), two-dimensional experiments, and efforts at the microscale are summarized. These particular areas are chosen for two reasons. First, these areas represent the tasks for which the most significant progress has been achieved. Second, these areas are critical to successful continuation of this project. Third, these three areas represent the three general thrusts of this work, namely experiments on porous media, innovation in experimental design, and analysis of microscopic behavior.

Advances in Experimental Design

Substantial effort has been placed in the advancement of the experimental design utilized in these experiments. Principal among the scientific advancements has been the development of an inexpensive flow cell, development of a flow cell for converging / diverging flow and a carrying fluid which can be frozen *in situ*.

The primary advantages of the flow cell design discussed previously over previous designs utilized within the SSP include the low cost of each cell, the flexibility of design for each cell, and the clear surfaces along all faces of the cell. The primary disadvantages are the failure of these cells after repeated use (as compared to designs constructed from stainless steel), the use of silicon sealants, and the potential for biological contamination along the seams of the cell. We consider this modification of the flow cell design to be significant for the SSP in terms of expanding the use of intermediate-scale studies, but we do not consider this to be a fundamental scientific advancement which requires further discussion in this section of the packet.

The flow cell design for the converging / diverging flow fields, however, is considered to be a fundamentally new concept in intermediate scale study which may have significant scientific impact. As stated earlier, the final details of the design are not yet complete as testing of the initial design continues. However, a schematic of the general details of the design is given in Figure 4. The cell design allows injection or withdrawal of fluid from the central "well" with simultaneous withdrawal or injection along the outer ring. Both the inner well and the outer ring consist of standard well screen (1" and 24" diameter, respectively) with 0.008" slots. The outer reservoir is mixed through recirculation pumps to reduce concentration gradients (chemical and particle) within this reservoir. This design also allows the outer reservoir to be subdivided should there be a need to modify injection or withdrawal rates as a function of angle along this boundary.

This design is a modification of a design suggestion by Dr. James Szecsody (PNL) in which he suggested a pie shaped flow cell. This design was chosen over the pie shaped cell for three reasons. First, this design allows unrestricted flow along any arch within the medium (whereas the pie shaped cell required imposition of no flow boundaries along the edge radii of the cell). Second, this cell appears simpler to construct and operate than the pie shape cell as there are no awkward angles to deal with at the location of the inner well. Finally, this cell opens the potential for substantially new experiments in hydraulics and transport within a flow regime with significant similarity to those encountered in many field operations for which injection or withdrawal from a well is required. For these reasons, we believe that this flow cell design is a scientific advance of importance at a fundamental level as it provides an opportunity to pursue fundamentally different experiments within the laboratory.

Figure 4: Schematic of General Design: Converging / Diverging Flow Cell

The UV curing resin holds great promise in advancing experimental efforts in saturated and unsaturated media. The resin used is a 2000 series clear, deep-curing resin purchased from the Polychem Corporation (Cranston, Rhode Island). The resin has a viscosity of 200 cps at 75°F and a specific gravity at 20°C of 1.10. The resin is reported to act as a Newtonian fluid. Curing time is reported as 5 seconds under a UV source measuring 10,000 mw/cm².

The viscosity of the resin is sensitive to temperature (we observed a change of nearly 20% in viscosity as the temperature of the resin was varied from 25°C to 31°C). We have used a focused source of UV light with a strength of approximately 1,000 mw/cm² (UVEX model SCU110, UVEX, Sunnyvale, California) for all curing. The wand through which the UV light passes is 8 mm in diameter. Curing has been performed through direct exposure of the resin, through glass, through 1.2 centimeter thick plexiglass, and through glass rods with a 1 millimeter O.D. Curing time and curing depth are functions of the area of exposure and the type of medium through which the UV light must pass. Exposure of the resin (which was distributed within the pores of #10 sieve glass beads) to UV light directly from the UVEX wand for a period of 10 seconds produced a cured volume of resin and glass beads of approximately 8 cubic centimeters. Exposure of resin within the pore space of #10 sieve glass beads via 1 millimeter diameter glass rods for periods of approximately 60 seconds produced a layer of cured resin and glass beads

along all exposed surfaces of the glass rod plus a volume of cured resin and glass beads of approximately 2 cubic centimeter at the tip of the glass rod.

The resin cures to a transparent solid with little distortion with respect to light transmission. Curing the resin within a glass bead medium leads to relatively weak bonds with the glass beads, allowing easy removal of beads for inspection of bead/resin contacts. However, these relatively weak bonds may lead to difficulty in thin sectioning the resin/bead mixture. In addition, the resin tends to crack along irregular surfaces, making microscopic analysis of simply cracked specimens subject to some distortion due to the light refraction at these surfaces. Despite these difficulties, microphotographs of cured specimens can be accomplished.

Curing of the resin leads to slight reduction in volume. During our tests, the volume reduction during curing was approximately 1.4%. During curing through plexiglass, the resin does not appear to separate from the plexiglass as no liquid resin is observed to flow between the plexiglass and cured resin during flow experiments.

The curing process is strongly exothermic. We have run two types of experiments to characterize the temperature changes occurring during curing. In the first experiment, the resin was cured in an open container. The second experiment involved curing the resin which filled the pore spaces of a medium consisting of #10 sieve glass beads. For both experiments, the resin was exposed to UV light for approximately 60 seconds (substantially longer than required to achieve curing). The temperature increased substantially in both experiments with a maximum increase of approximately 50 °C for the first experiment and approximately 30 °C in the second experiment. The cured volume for the resin in the glass beads was larger than the cured volume in the open container. Despite the high temperatures generated during curing, the resin does not demonstrate any strong thermal conduction cells near the cure point, even in an open container of resin with a concentrated region of curing.

During a recent experiment in two-dimensions, the resin was used instead of water as the carrying fluid. A series of eight glass rods were inserted into the flow cell (prior to packing) with the tips of the rods exposed at the midpoint between the side walls of the cell. During the experiment, each rod was exposed to UV light for approximately 120 seconds at the time of expected arrival of the tracer front. After completion of the experiment (prior to opening the cell) additional locations were cured through exposure of the resin light through the plexiglass. Finally, after the flow cell was opened, selected uncured portions of the medium were sampled. Latex particles were clearly visible within the cured resin such that number and location could be identified under microscopic analysis.

The resin has performed extremely well in the initial test under experimental conditions. It is anticipated that increasing use will be made of the resin as experiments extend to three dimensions. In addition to this application to particle transport, the resin is proving useful for visualization and characterization of contact angles and moisture profiles in unsaturated media, for characterization of residual moisture and contact angles in multiphase flow, and in characterization of multiple scales of dispersion in the transport of dyes. A manuscript is currently in preparation describing these applications of the resin.

Results from Two-Dimensional Experiments in Saturated Media

A number of experiments have been conducted in two-dimensional porous media using both water and the UV resin as the saturating fluid (one fluid at a time). These experiments have included work in homogeneous glass beads, simple layers, slanted layers, simple heterogeneities

and complex heterogeneities. Due to limited space, the results discussed will be limited to two experiments in layered media and three experiments in more general heterogeneous conductivity distributions.

The first experiment consisted of layers aligned parallel with the primary flow direction such that flow entering one layer remained in that layer from inflow to outflow. The medium in this case consisted of approximately 10% coarse beads, 25% medium beads and the remainder small diameter glass beads. The second medium consisted of the same mixture of beads, but the layers were angled such that all flow was required to pass through a minimum of 5 centimeters of the small glass beads. The three heterogeneous media discussed were shown previously in Figure 2. Water (with sodium chloride added to increase the density to 1.05 g/cc) was used as the carrying fluid in the first four experiments while the UV resin was used in the final experiment (the lower most pattern in Figure 2).

In all cases in which water was used as the carrying fluid, latex spheres were found in high concentration within the medium despite flushing the medium for a minimum of the time required to drive the outflow concentration of particles to zero. In experimental work on the homogeneous glass beads, it was determined that particles were always found in relatively large numbers within the medium despite significant flushing and a change in ionic strength from the original water (density of 1.05 g/cc) to water directly from our reverse osmosis unit. In fact, contrary to some earlier work on colloid transport through glass beads, we did not see a release of latex spheres when the ionic strength of the carrying fluid was lowered. In contrast to these results, when we utilized the UV resin as the carrying fluid (higher viscosity and different chemistry), very few to zero latex spheres were located within the structure of the medium after the experiment (except for those contained in the locations cured during the experiment). This result provides an initial indication that the loss of latex particles to the medium in these experiments is largely a function of trapping and that this loss may be altered through adjustment of the shear stress and/or by providing a path of travel along which the latex particle does not change conductivity regions.

This latter suggestion is derived from an analysis of the location of particles remaining within the medium after each of the experiments. As demonstrated in Figure 5, the concentration of particles remaining within the medium tends to decrease with distance from the inflow reservoir except where flowlines cross media boundaries (particularly high to low permeability). In this case, there appears to be an accumulation of latex spheres at and upstream from this boundary. This accumulation is indicated in the results for the slanted layers (top figure in Figure 5) for which the concentration of particles rises at and upstream of the boundaries between the coarse and medium glass beads and again at the boundary between the medium and fine glass beads. This observation is supported by the majority of our results (e.g. the lower figure in Figure 5), but the interpretation is often difficult due to the complex heterogeneities in some experiments.

In addition to the loss of particles within the medium, there is also a separation of particles within the medium. In all cases, the larger particles are preferentially lost to the medium during transport. That is, the small particles are usually under represented in the particles remaining in the media at the end of the experiments. Finally, Figure 6 shows that for those systems in which the particles had direct flow paths through the medium without a requirement of motion through the fine glass beads, breakthrough of all particle sizes was observed in relatively large concentration. When flow was forced to move through the fine glass beads or when the flow path was very tortuous, the latex particles did not tend to flow through the medium (outflow concentrations were very small and consisted primarily of small particles).

These results have been presented at AGU and are being prepared for publication.

Figure 5: Concentration of Latex Particles Remaining in Medium at End of Experiment for Slanted Layer System (top) and Simple Heterogeneous System (Bottom). Counts Shown have not yet been Converted to Counts/Milliliter. However, a Count of 100 Coincides with Approximately 7,500 Counts per Milliliter. Inflow Counts Were Approximately 150,000 Counts/Milliliter for the Top Experiment and Approximately 30,000 Counts per Milliliter for the Lower Experiment.

Figure 6: Outflow Particle Counts for the Five Experiments Discussed. Failure of Particles to Cross the Medium in the Slanted Layers and the Complex Heterogeneity is Thought to be Related to Flow Through the Fine Beads and/or Tortuosity of the Flow Path. A Count of 100 is Equivalent to Approximately 7500 Counts per Milliliter.

Results From Numerical Efforts

The theoretical efforts have produced results in three general areas. First, in terms of characterization of dispersion in the simulated fields, substantial theoretical advances have been realized. Following Mei (1993), it is possible to formulate a boundary value problem (BVP) for an auxiliary vector variable N_i on the unit periodic cell. Equations for each component of N_j are similar to the original advection-diffusion equation but contain a source term related to the deviations of point velocities from the mean. After averaging, the concentration is found to obey the regular advection-dispersion equation at the macroscale. The dispersion tensor which appears in this equation can be obtained by averaging from the solution of the BVP for N_j . A numerical model was developed for solution of the BVP described above. The model is based on the FTCS finite-difference scheme. The steady solution of the BVP is obtained as an asymptotic solution of the unsteady problem. The solution is found to depend on the Peclet number and the properties of the porous media (porosity, correlation function) as well as on the size of the unit periodic cell. The summary of results for a twenty by twenty field with the porosity of 0.75 is presented in Figure 7. The figure shows that the dispersion coefficient increases with the Peclet number. This result is in a good qualitative agreement with results reported in the literature. The limitation of the present numerical model is imposed by the computational requirement that the cell Peclet number, defined as $Pe_c = U\Delta x/D$, be less than four. This in turn poses restrictions on the upper limit of values of the dispersion coefficient that can be obtained within available computational resources. This theoretical effort is currently being prepared for publication.

Second, results of the solution of the Navier-Stokes equation combined with verification using the Hele-Shaw cell have led to a number of interesting results. The Marker and Cell (MAC) model was initially tested on flow between parallel plates without obstructions and flow between parallel plates with a single obstruction. Comparison with analytical solutions for these two problems demonstrated that the model was working efficiently. Simulations were then extended to a series of 10 simulations each for internal porosities ranging from 60% to 90% in 5% increments. From these results, a relation between the hydraulic conductivity of the idealized porous medium and the field's porosity was obtained. This relationship is shown in Figure 8.

The MAC model was also used to define streaklines in a small number of simulations for direct comparison with results from the Hele-Shaw laboratory model. Qualitative comparison of the numerical and experimental results is very promising. Work on these comparisons continues, but an initial paper on both this aspect and the permeability relationship is in preparation.

Third, results from the Monte Carlo simulations have provided interesting initial results. Working on media in which the correlation length scale is large in comparison to the length scale of transport, the difference in mean travel time and variation in travel time between discrete random fields and continuously varying random fields is significant. However, when the correlation length scale is small, the difference in mean and variance of travel time is negligible. Work continues to further confirm these conclusions and to extend results into consideration of capture zone geometries. Two presentations at AGU were derived from these efforts.

Figure 7. Ratio of the longitudinal dispersion coefficient and the molecular diffusion coefficient versus the Peclet number as obtained from the solution of the BVP posed by the homogenization method.

Figure 8. Dimensionless permeability versus the porosity as obtained from the solution of the Navier-Stokes equations by the MAC method. Circles: calculated points; solid line: average of 10 realizations per porosity; dashed lines: one standard deviation envelope.

REFERENCES

- Harvey, R.W., N.E. Kinner, D. MacDonald, D.W. Metge, and A. Bunn, "Role of physical heterogeneity in the interpretation of small-scale laboratory and field observations of bacteria, microbial-sized microsphere, and bromide transport through aquifer sediments", *Water Resources Research*, 29(8), 2713-2721, 1993.
- Harvey, R.W., L.H. George, R.L. Smith, and D.R. LeBlanc, "Transport of microspheres and indigenous bacteria through a sandy aquifer: Results of natural and forced-gradient tracer experiments", *Environ. Sci. Tech.*, 23, 51-56, 1989.
- McCarthy, J.F. and C. Degueldre, "Sampling and characterization of colloids and particles in groundwater for studying their role in contaminant transport", in *Environmental Particles*, Vol.2, Lewis Publishers, Ann Arbor, 247-315, 1993.
- McCarthy, J.F. and J.M. Zachara, "Subsurface transport of contaminants", *Environmental Science Technology*, 23(5), 496-504, 1989.
- McDowell-Boyer, I.M., J.R. Hunt, and N. Sitar, "Partical transport through porous media", *Water Resources Research*, 22(13): 1901-1921, 1986.
- Mei, C.C., "Method of homogenization applied to dispersion in porous media", *Transport in Porous Media*, 9, 261-274, 1992.
- Mills, W.B., S. Liu, and F.K. Fong, "Literature review and model (COMET) for colloid/metals transport in porous media", *Ground Water*, 29(2), 199-208, 1991.
- Mills, A.L., G.M. Hornberger, J.S. Herman, J.E. Sqiers and D.E. Fontes, "Bacterial transport in heterogeneous porous media", *First international symposium on deep subsurface microbiology*, Orlando, 1990.
- Silliman, S.E., "The influence of grid discretization on the percolation probability within discrete random fields", *Journal of Hydrology*, 113, 177-191, 1990.
- Wilson, J.L., J. Wan, and T. Nowicki, "Microscopy of micro-organism transport in an artificial porous matrix", *EOS*, 74(16), 132, 1993.

DATE

FILMED

1 / 21 / 94

END

_____

_____